

## I U C L I D

## Data Set

## Robust Summaries

Existing Chemical : ID: 80-51-3  
CAS No. : 80-51-3  
EINECS Name : 4,4'-oxydi(benzenesulphonohydrazide)  
EC No. : 201-286-1  
Molecular Formula : C12H14N4O5S2

Status :  
Memo : Celogen OT Crompton US HPV

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Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

RECEIVED  
OPT CDIC  
2003 SEP -3 AM 11:46

## 2. Physico-Chemical Data

Id 80-51-3  
Date 19.05.2003

### 2.1 MELTING POINT

Decomposition : yes, at 150 - 160 °C  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Reliability : (1) valid without restriction  
Peer reviewed literature

17.03.2003

(3)

### 2.2 BOILING POINT

Decomposition : yes  
Year :  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Remark : Decomposes prior to melting

17.03.2003

(3)

### 2.4 VAPOUR PRESSURE

Value : .0000000000089 hPa at 25 °C  
Decomposition :  
Method : other (calculated): MPBPWIN v1.40  
Year : 2003  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)

26.03.2003

(6)

### 2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water  
Log pow : .08 at °C  
pH value :  
Method : other (calculated): KOWWIN v1.66  
Year : 2003  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Reliability : (2) valid with restrictions

26.03.2003

(6)

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water  
Value : 4733 mg/l at °C  
pH value :  
concentration : at °C  
Temperature effects :  
Examine different pol. :  
pKa : at 25 °C  
Description :  
Stable :  
Deg. product :  
Method : other: Calculated using WSKOW v1.40  
Year :  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Reliability : (2) valid with restrictions

26.03.2003

(6)

## 3.1.1 PHOTODEGRADATION

Type : air  
Light source :  
Light spectrum : nm  
Relative intensity : based on intensity of sunlight  
INDIRECT PHOTOLYSIS  
Halflife t1/2 : 61 hour(s)  
Degradation : % after  
Quantum yield :  
Deg. product :  
Method : other (calculated): AOPWIN v1.90  
Year : 2003  
GLP :  
Test substance :  
  
Remark : Concentration of hydroxyl radicals in air = 1.5E6 OH/cm3  
12-hour day  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Reliability : (2) valid with restrictions  
26.03.2003

(6)

## 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III  
Media :  
Air : % (Fugacity Model Level I)  
Water : % (Fugacity Model Level I)  
Soil : % (Fugacity Model Level I)  
Biota : % (Fugacity Model Level II/III)  
Soil : % (Fugacity Model Level II/III)  
Method : other: calculation using Epiwin Level III Fugacity Model  
Year : 2003  
  
Test condition : Henry's Law Constant: 1.26E-17 atm-m3/mole (Henrywin program)  
Vapor pressure: 6.67E-12 mmHg (Mpbpwin program)  
Log Kow: 0.08 (KOWWIN program)  
Soil Koc: 0.493 (calc by model)  
Melting point: 237 °C (MpBpwin program)  
  
1000 kg/hr emissions to air, water and soil compartments.  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Attached document : Fugacity Model Data.doc

	Mass Amount (percent)	Half-life (hr)	Emissions (kg/hr)
Air	2.35E-7	122	1000
Water	49.1	900	1000
Soil	50.8	900	1000
Sediment	0.0916	3.6E+3	0

Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
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### 3. Environmental Fate and Pathways

Id 80-51-3  
Date 19.05.2003

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Air	3.52E-21	3.17E-5	5.59E-5	1.06E-6	1.86E-6
Water	2.05E-22	900	1.17E+3	30	39
Soil	7.57E-21	931	0	31	0
Sediment	1.89E-22	0.42	0.0436	0.014	0.00145

Persistence time: 793 hr  
Reaction time: 1.3E+3 hr  
Advection time: 2.04E+3 hr  
Percent reacted: 61  
Percent advected: 39

Half-lives (hr), (based upon Biowin (ultimate) and Aopwin):

Air: 122  
Water: 900  
Soil: 900  
Sediment: 3600  
Biowin estimate: 2.349 (weeks-months)

Advection times (hr):

Air: 100  
Water: 1000  
Sediment: 5E+4

**Reliability** : (1) valid without restriction  
26.03.2003

(6)

#### 3.5 BIODEGRADATION

**Type** : aerobic  
**Inoculum** :  
**Deg. product** :  
**Method** : other: Estimation using BIOWIN v4.00  
**Year** : 2003  
**GLP** :  
**Test substance** : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
**Result** : MITI linear biodegradation probability = -0.466  
MITI non-linear biodegradation probability = 0.000

Not Readily biodegradable  
**Reliability** : (2) valid with restrictions  
26.03.2003

(6)

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type :  
Species :  
Exposure period : 96 hour(s)  
Unit : mg/l  
LC50 : 9.76  
Method : other: calculation using Ecosar v0.99g  
Year : 2003  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Test condition : Log Kow: 0.08 (KowWin estimate)  
Water solubility: 1.45E+5 (calculated)  
Ecosar class: Hydrazines  
Reliability : (2) valid with restrictions  
26.03.2003

(6)

## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :  
Species : Daphnia sp. (Crustacea)  
Exposure period : 48 hour(s)  
Unit : mg/l  
EC50 : 17.37  
Method : other: calculation using Ecosar v0.99g  
Year : 2003  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Test condition : Log Kow: 0.08 (KowWin estimate)  
Water solubility: 1.45E+5 (calculated)  
Ecosar class: Hydrazines  
Reliability : (2) valid with restrictions  
26.03.2003

(6)

## 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species :  
Endpoint :  
Exposure period : 144 hour(s)  
Unit : mg/l  
EC50 : 2.36  
Method : other: calculation using Ecosar v0.99g  
Year : 2003  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Test condition : Log Kow: 0.08 (KowWin estimate)  
Water solubility: 1.45E+5 (calculated)  
Ecosar class: Hydrazines  
Reliability : (2) valid with restrictions  
26.03.2003

(6)

## 5. Toxicity

Id 80-51-3

Date 19.05.2003

### 5.1.1 ACUTE ORAL TOXICITY

Type : LD50  
Value : > 5200 mg/kg bw  
Species : rat  
Strain : other: albino  
Sex : no data  
Number of animals :  
Vehicle : other: olive oil  
Doses : Maximum dose was 9 cc of a 14.3% solution  
Method : other: United States Testing Co., Inc method  
Year : 1950  
GLP : no  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Supplier: Naugatuck Chemical Co.  
Lot No: ILGE A-2609  
Purity: No data  
Method : Post dose observation period: 3 days  
Result : The minimum oral LD50 of a compound is the minimum dose which may be expected to kill half of the animals in a test group upon oral administration. In this study, an oral LD50 was not obtainable at the highest level fed.  
  
The highest level fed was equivalent to 1.3g of the sample for rats weighing approximately 250 g, i.e. 5200 mg/kg.  
Reliability : (2) valid with restrictions  
27.03.2003 (5)

Type : LD50  
Value : 2300 mg/kg bw  
Species : rat  
Strain :  
Sex :  
Number of animals :  
Vehicle :  
Doses :  
Method : Unknown  
Year : 2002  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Purity: No data  
Reliability : (4) not assignable  
23.06.2003 (7)

### 5.1.3 ACUTE DERMAL TOXICITY

Type :  
Value :  
Species : rabbit  
Strain :  
Sex :  
Number of animals : 10  
Vehicle : water  
Doses : 200 mg/kg  
Method : other: FIFRA Section 162.8 (c), March 1948  
Year : 1950

## 5. Toxicity

Id 80-51-3  
Date 19.05.2003

**GLP** : no  
**Test substance** : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Supplier: Naugatuck Chemical Co.  
Lot No: ILGE A-2609  
Purity: No data  
**Method** : The calculated dosage was first dissolved in distilled water and then placed onto gauze squares. The squares were immediately placed on the bare skin of each rabbit and securely held in place with waterproof adhesive tape. Care was taken to completely cover each patch securely so as to minimize evaporation and to insure continuous contact with the skin for 24 hours.  
**Result** : The following observations were made after 24 hours:  
  
1. All animals were alive and well after the 24 hour period  
  
2. No toxic manifestations were exhibited by any of the animals under test.  
**Reliability** : (2) valid with restrictions  
27.03.2003 (5)

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

**Type** : LD50  
**Value** : > 5000 mg/kg bw  
**Species** : mouse  
**Strain** :  
**Sex** : no data  
**Number of animals** :  
**Vehicle** : physiol. saline  
**Doses** : up to 2.5 c.c. of a 5% solution  
**Route of admin.** : i.p.  
**Exposure time** :  
**Method** : other: United States Testing Co., Inc method  
**Year** : 1950  
**GLP** : no  
**Test substance** : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Supplier: Naugatuck Chemical Co.  
Lot No: ILGE A-2609  
Purity: No data  
**Method** : Post dose observation period: 3 days  
**Result** : Unable to obtain a definite killing point.  
  
The highest concentration injected was equivalent to 5000 mg/kg b.w.  
**Reliability** : (4) not assignable  
27.03.2003 (5)

### 5.2.1 SKIN IRRITATION

**Species** : rabbit  
**Concentration** : 50 mg  
**Exposure** :  
**Exposure time** : 24 hours  
**Number of animals** :  
**Vehicle** : other  
**PDII** :  
**Result** :  
**Classification** :  
**Method** : EPA OPP 81-5  
**Year** : 1950

## 5. Toxicity

Id 80-51-3

Date 19.05.2003

GLP : no  
Test substance : As prescribed by 1.1-1.4  
Method : 50 mg of the sample was mixed with Vaseline and placed on to gauze squares, which were then placed on the bare skin of rabbits. The squares were held in place by waterproof adhesive tape. This test was conducted on 3 rabbits. As a control the effect of pure Vaseline was tested in a similar manner. The patches were removed 24 hours later and the skin was observed for signs of irritation  
Result : Slight reaction was observed in the treated rabbits and there was no irritation seen in the control  
Reliability : (4) not assignable  
23.07.2003 (7)

Species : rabbit  
Concentration :  
Exposure :  
Exposure time :  
Number of animals : 3  
Vehicle : physiol. saline  
PDII :  
Result :  
Classification :  
Method : other: United States Testing Co., Inc method  
Year : 1950  
GLP : no  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Supplier: Naugatuck Chemical Co.  
Lot No: ILGE A-2609  
Purity: No data  
Method : The test substance was extracted in 5% amounts in physiological saline in an autoclave. The extracts were then injected with aseptic precautions into the rabbits. Ater 24 hours the rabbits were observed for presence of irritation.  
Result : There was a slight reaction caused by the extracts of the sample.  
Reliability : (4) not assignable  
27.03.2003 (5)

### 5.4 REPEATED DOSE TOXICITY

Type :  
Species : rat  
Sex : male/female  
Strain :  
Route of admin. : oral feed  
Exposure period : 90 days  
Frequency of treatm. : daily  
Post exposure period :  
Doses : 20 ppm (1mg/kg bw/day), 2000 ppm (100 mg/kg bw/day)  
Control group :  
Method :  
Year : 1981  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Remark : This study is limited because a restricted range of tissues of only half of any group of treated animals were subject to detailed microscopic examination.  
Result : NOEL = 1 mg/kg bw/day



## 5. Toxicity

Id 80-51-3

Date 19.05.2003

Groups of 12 rats of each sex fed diets containing 2000 ppm (100 mg/kg bw/day) for 90 days showed reduced food consumption and depressed growth, and two of the male rats died within 10 weeks appearing malnourished. Increased liver and kidney weights were noted, but no macroscopic abnormalities or effects on the blood were seen in the surviving animals. These findings were attributed by the investigators to the low palatability of the diet. No effects were observed in animals fed 20 ppm (1 mg/kg bw/day).

**Reliability** : (4) not assignable  
16.05.2003 (1)

**Type** :  
**Species** : rat  
**Sex** :  
**Strain** :  
**Route of admin.** : gavage  
**Exposure period** : 4 months  
**Frequency of treatm.** : daily  
**Post exposure period** :  
**Doses** :  
**Control group** :  
**LOAEL** : 36 mg/kg bw  
**Method** :  
**Year** : 1969  
**GLP** :  
**Test substance** : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
**Result** : Doses of approximately 200 mg/kg bw/day by stomach tube killed all six rats within 2 weeks. Growth was reduced in six rats given 36 mg/kg bw/day by stomach tube for 4 months. Increased liver weight, disturbance of liver and kidney function and changes in the appearance of the liver, kidney and adrenals were also seen.

**Reliability** : (4) not assignable  
16.05.2003 (4)

### 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : Chromosome aberration test  
**System of testing** :  
**Test concentration** :  
**Cycotoxic concentr.** :  
**Metabolic activation** :  
**Result** : Negative

The results indicate that the test substance did not cause a statistically significant increase in the number of chromosome aberrations ( $p < 0.05$ ). This was observed for both activated and non-activated systems. In addition, there was no detectable dose response in the number of aberrations of both activated and non-activated systems, verifying the validity of the test system. In conclusion, the test substance did not induce chromosomal aberrations in Primary Cultured Human Lymphocytes and is considered non-clastogenic

<b>Method</b>	: The test substance was evaluated for its ability to induce chromosomal aberrations in primary human lymphocyte cells in the presence and absence of a rat liver homogenate metabolic activation system. The test article was tested at the following concentrations: Neat and 1:2, 1:4, 1:8, 1:16, 1:32 and 1:64 dilutions of the neat extract. The concentrations chosen to be scored for the activated assay were Neat and 1:2 and 1:4 dilutions of the test extract. The following controls were used: 1. Negative Control Article:- RPMI Cell Culture medium, the extraction vehicle, served as the negative control article. 2. Positive Control Article (Non-activated system):- Mitomycin C (MMC) is a known mutagen and clastogenic agent and served as the positive control article for the non activation system. 3. Positive Control Article (Activated System):- Cyclophosphamide (CP) is a clastogen that requires metabolic transformation by microsomal enzymes. It served as the positive control article for the activation assay
<b>Year</b>	: 1997
<b>GLP</b>	:
<b>Test substance</b>	: 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3) Purity: no data
<b>Reliability</b> 23.06.2003	: (4) not assignable
	(7)
<b>Type</b>	: Bacterial reverse mutation assay
<b>System of testing</b>	:
<b>Test concentration</b>	: Neat, 1:2, 1:4, 1:8 and 1:20 fold dilutions.
<b>Cycotoxic concentr.</b>	:
<b>Metabolic activation</b>	: +/-
<b>Result</b>	: Positive
<b>Method</b>	: EPA OTS 798.5265
<b>Year</b>	: 1997
<b>GLP</b>	: Yes
<b>Test substance</b>	: 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3) Purity: no data
<b>Method</b>	: The Salmonella typhimurium Reverse Mutation Assay (Ames Assay) test was conducted to evaluate the potential for the test substance to induce histidine reversion caused by base changes or frameshift mutations in the genome of this organism. The direct plate incorporation assay was conducted with four strains of Salmonella typhimurium in the presence and absence of exogenous mammalian activation system.
<b>Result</b>	: The test substance is mutagenic.
<b>Reliability</b> 23.06.2003	: (4) not assignable
	(7)
<b>Type</b>	: Bacterial reverse mutation assay
<b>System of testing</b>	:
<b>Test concentration</b>	:
<b>Cycotoxic concentr.</b>	:
<b>Metabolic activation</b>	:
<b>Result</b>	: positive
<b>Method</b>	:
<b>Year</b>	:
<b>GLP</b>	:
<b>Test substance</b>	: 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3) Purity: no data
<b>Remark</b>	: 4,4'-Oxybis(benzenesulphonyl hydrazide) was mutagenic in Salmonella typhimurium (Ames test) in the presence or absence of a liver metabolic activation system (Hachiya, 1987; Shimizu, 1986; Shimizu et al, 1978). In a test with one strain of Escherichia coli, a liver metabolic activation system

## 5. Toxicity

Id 80-51-3  
Date 19.05.2003

was required for the hydrazide to exhibit mutagenic potential (Shimizu, 1986), although tests with other strains (Hachiya, 1987; Shimizu, 1986), found no evidence of mutagenicity in the presence or absence of a liver metabolic fraction.

Reliability : (4) not assignable  
16.05.2003 (2)

### 5.6 GENETIC TOXICITY 'IN VIVO'

Type : Micronucleus assay  
Species :  
Sex :  
Strain :  
Route of admin. :  
Exposure period :  
Doses :  
Result : Negative  
Method :  
Year :  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Purity: no data  
Reliability : (4) not assignable  
23.06.2003 (7)

Type : Unscheduled DNA synthesis  
Species :  
Sex :  
Strain :  
Route of admin. :  
Exposure period :  
Doses :  
Result : Negative  
Method :  
Year :  
GLP :  
Test substance : 4, 4'-oxydi(benzenesulfonohydrazide) (CAS No. 80-51-3)  
Purity: no data  
Reliability : (4) not assignable  
23.06.2003 (7)

#### 5.8.1 TOXICITY TO FERTILITY

#### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

- (1) Borgstedt, H.H. (1981). 90-day feeding study in rats. Final report volume 1. Department of Pharmacology & Toxicology. University of Rochester. USA; reported in BIBRA International Ltd (1997). Toxicity Profile for 4,4'-Oxybis(benzenesulphonylhydrazide)
- (2) Hachiya, N. (1987). Akita J. Med. 14 269; Shimizu, H. (1986). Tokyo Jikeika med. J. 101, 167; Shimizu, H. et al (1978) Jpn J. Hygiene 33, 474; reported in BIBRA International Ltd (1997). Toxicity Profile for 4,4'-Oxybis(benzenesulphonylhydrazide)
- (3) Hawley, G.G., The Condensed Chemical Dictionary, 9th ed., New York, Nostrand Rheinhold Co., p 643, 1977
- (4) Shurupova, G.A., et al (1969). Sin. Issled Eff. Khimikatov. Polim. Mater. 3, 438; reported in BIBRA International Ltd (1997). Toxicity Profile for 4,4'-Oxybis(benzenesulphonylhydrazide)
- (5) United States Testing Company, Inc, Test Report 21672, July 21, 1950
- (6) US EPA, EPIWIN v3.10, EPI Suite Software, 2000
- (7) IUCLID Dataset for Existing Chemicals, 4, 4'-oxydi(benzenesulfonohydrazide), 2002